Discovery at the Interface of Science and Engineering: Science Matters!

Engineering Sciences
Structural Mechanics

Coupled Multi-Physics Modeling to Support Energy R&D

Physical and chemical processes due to the burial of high-level radioactive waste can be simulated in greater detail with new engineering codes.

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Geologic repositories have played a critical role in US energy policy for several decades. The recent expansion of the Strategic Petroleum Reserve and the on-going operation of the Waste Isolation Pilot Plant to permanently dispose of low-level radioactive waste are prime examples of successful engineering of geologic systems to address critical national needs. These successes have fueled interest in developing other geologic systems for more challenging national energy problems, including high level nuclear waste disposal (Figure 1), compressed air methods for retrievable energy storage, utilizing geothermal energy, and CO_2 sequestration.

Development of long-term solutions to these needs requires the ability to model, simulate, and predict behavior of subsurface systems over geologic time scales. These behaviors include complex, heterogeneous mineral and porous rock thermo-chemo-mechanical behavior as well as the interactions with multi-phase pore fluids and microbial activity. Recent investments by Sandia in the SIERRA Mechanics code suite provide the basic building blocks for realizing this multi-physics capability for geosystems engineering: fluid flow, nonlinear geomechanics, geochemistry, heat transfer, etc., with an application focus on CO_2 sequestration and radioactive waste disposal. This research has benefitted from collaborations with the University of Texas at Austin Center for Subsurface Modeling, and from interactions with the Center for Frontiers of Subsurface Energy Security which is an Office of Basic Energy Sciences Energy Frontier Research Center.

Here is shown how this modeling was recently applied in a feasibility analysis of high-level radioactive waste disposal in a clay/shale medium. A three-dimensional analysis of a section of a clay/shale waste repository is shown in Figure 1. The waste is stored in an unlined horizontal borehole

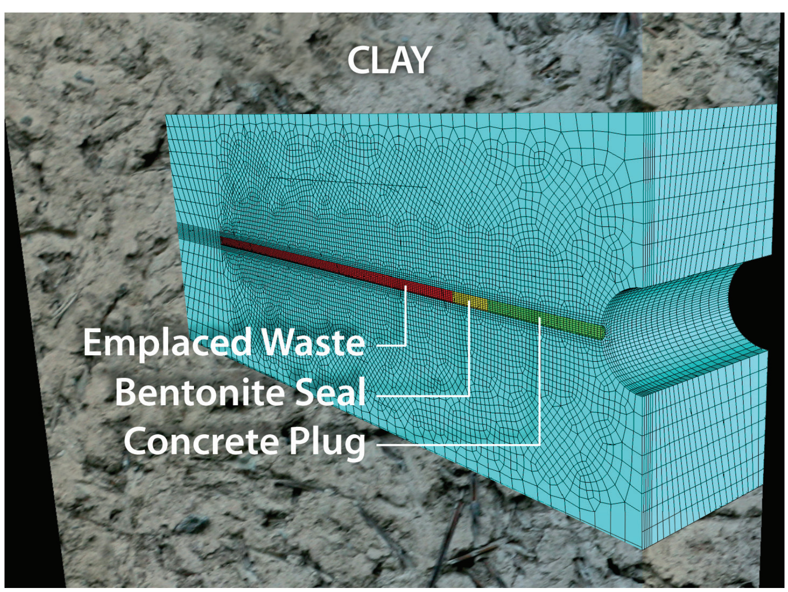

Figure 1: Clay/shale waste repository geometry with the finite element discretization showing the location of the emplaced waste, concrete, and bentonite plug.

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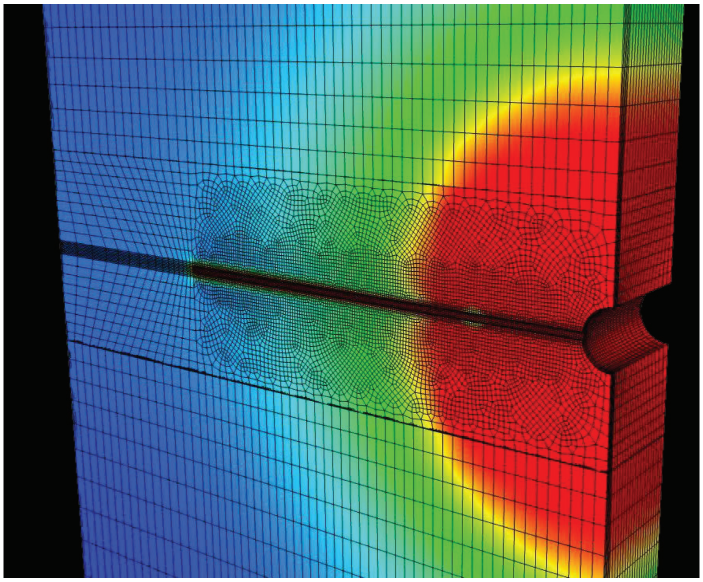

Figure 2: Region of assumed damage in the clay/shale after excavation. Red is a region of highest damage.

perpendicular to the main access tunnel. The disposal borehole would be sealed at the end with concrete and bentonite (a form of clay) plugs. The multi-physics approach was needed due to a coupling between the high heat generated by the radioactive waste, the presence of water, and the dependence of clay/shale strength and deformability on the water content. Moreover, since thermally-driven fluid movement may transport radionuclides away from the waste source, species transport was included in the analysis.

Figure 2 shows the region of damage that results due to the initial excavation of the access tunnel and borehole, where red indicates a possible increase in local clay/shale porosity and permeability. Fractures and voids that form during excavation will eventually heal over time due to the sealing nature of the clay. However, peak emplacement borehole temperatures can range from 83 ºC for typical high-level waste power densities to greater than 200 ºC for some very high-level wastes. The simulation shows that the heat results in water evaporation in the repository near the emplacement boreholes (Figure 3). The extent of dessication also depends strongly on ambient rock permeability and, in some clays, will persist for a few thousand years. In contrast, high temperatures in combination with ultra-low rock permeabilities can trap high pressure superheated water vapor, potentially damaging the repository.

It has been shown in this waste repository example that the multiphysics capability in SIERRA Mechanics can model first-order interactions between important thermal, hydrological, and chemical processes. The development of the modeling capability has provided Sandia's scientists and engineers a new tool for modeling complex subsurface behavior and is currently being used to address other important areas of energy research such as CO_2 sequestration.

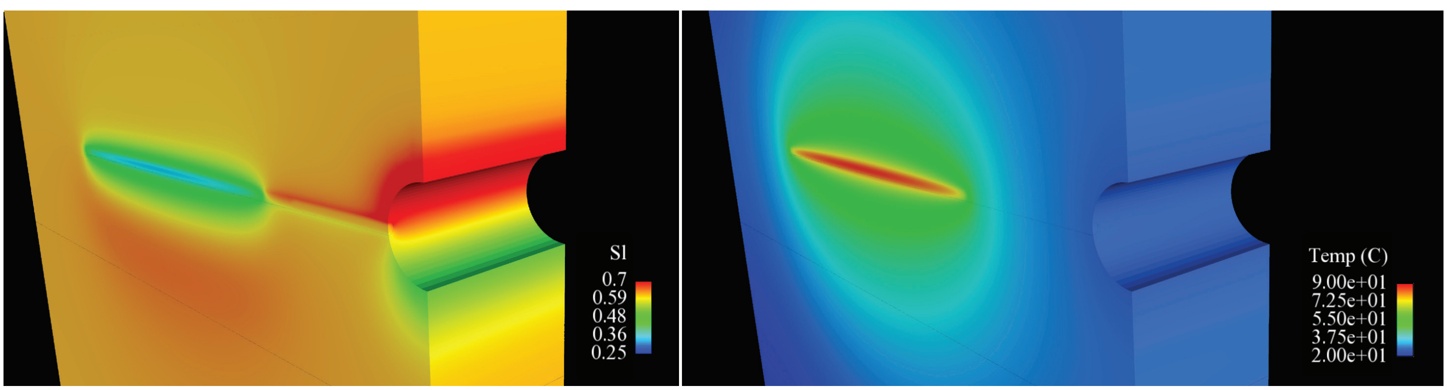

Figure 3: Water saturation (left) and temperature (right) contours near the waste horizon. Radioactive waste with high thermal output can produce dry out regions.

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